HYDROGEOPHYSICAL PARAMETER ESTIMATION APPROACHES FOR FIELD SCALE CHARACTERIZATION

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Abstract: Combinations of hydrogeological and geophysical data are increasingly used in hydrogeological site characterization. Although a wide range of methods to combine hydrogeological and geophysical data are presented in the literature, most investigations focus on development or application of a single method, and there have been few attempts to compare different methods. Here we review the choices that must be made in any hydrogeophysical parameter estimation effort, including model parameterization, the petrophysical relationship, and a-priori information. We distinguish between three classes of hydrogeophysical parameter estimation: direct mapping; integration methods; and joint inversion methods. We provide five examples that illustrate the different merits of those classes of methods. We conclude that direct mapping and integration methods, such as co-kriging, have proven their worth in hydrogeophysical parameter estimation. However, we argue that joint inversion methods might provide fundamental improvements because such methods facilitate information sharing and they form a consistent framework for addressing uncertainty and the worth of different data types.

Key words: inversion, hydrogeological parameter estimation, hydrogeophysics, a-priori information, regularization, integration methods, stochastic inversion.

1.1 Introduction

The potential benefits of including geophysical data in hydrogeological site characterization have been stated numerous times (e.g., Ezzedine et al., 1999; Hubbard et al., 1999; Chen et al., 2001; Hubbard and Rubin, 2005). The principle reason for the growing interest in using geophysical methods in hydrogeological studies is that geophysics may provide spatially distributed models of physical properties in regions that are difficult to sample using conventional hydrological wellbore methods (e.g., Butler, 2004). The geophysical models often reveal more details compared with hydrogeological estimates derived from hydrogeological data, such as pump tests and observations of hydraulic heads. Furthermore, geophysical methods are less invasive compared with hydrogeological methods and they are comparatively cheap. Therefore, geophysical surveys can improve hydrogeological characterization if we could relate the geophysical and hydrogeological properties in an appropriate way. The added value of including geophysics in hydrogeological characterization has become increasingly accepted and several published case studies clearly show the worth of including geophysics for different applications and data types (e.g., see reviews by Hyndman and Tronicke, 2005; Goldman et al., 2005; Daniels et al., 2005). However, the success of a given hydrogeophysical case-study is dependent on many different factors and it is often difficult to develop an opinion a-priori about the applicability of a method at another site or for another application. Here, we discuss some of the choices that need to be considered in a characterization effort and point out similarities and fundamental differences between different hydrogeophysical approaches presented in the literature.

The integration of hydrogeological and geophysical data sets is a complex process that often entails consideration of several different factors, such as:

- the measurement support volume is dependent on the characterization method;
- the models have space-varying resolution that depend on the data type, survey design, geological characteristics, and other factors;
- the effects of measurement errors and simplified assumptions are difficult to assess;
- an infinite number of models can often explain a finite number of noisy data.

Because of non-uniqueness, we need to state a preference for a certain type of model (e.g., the smoothest, the least number of model parameters, etc.) and it is not always clear how this preference effect the outcome of an investigation. Our problem of hydrogeophysical parameter estimation is further complicated because relationships between geophysical and hydrogeological parameters are often:

- non-unique;
- poorly understood; and
- non-stationary.

Reviews of petrophysical relationships for hydrogeological investigations are given by Lesmes and Friedman (2005) and Pride (2005).

In section 1.2, we discuss some critical choices that should be considered prior to the hydrogeophysical parameter estimation effort, such as: project objectives and available data (section 1.2.1); model parameterization (section 1.2.2); petrophysical relationship (section 1.2.3); a-priori information (section 1.2.4); optimization or Monte Carlo methods (section 1.2.5), objective functions (section 1.2.6); and at which stage to establish the link between geophysics and hydrogeology (section 1.2.7). We discuss three categories of hydrogeophysical parameter estimation, which we refer to as direct mapping (section 1.3), integration methods (section 1.4), and joint inversion methods (section 1.5). We acknowledge that not all research falls cleanly into a single category. For example, McKenna and Poeter (1995) used a geostatistical indicator simulation to define zonation Nonetheless, we find that this classification scheme is useful for the purposes of this review, and we give several case-studies to illustrate the merits and limitations of these categories (section 1.3-1.5). We conclude this chapter with a summary and outlook discussion (section 1.6).

We hope that this chapter will help the reader in considering the factors important for hydrogeophysical characterization, and in developing a hydrogeophysical parameter estimation approach for their specific problem of interest.

1.2 Critical choices

Throughout this chapter we group available data into geophysical and hydrogeological data. These data are further grouped into measurements of system properties (e.g., permeability) and measurements of state variables (e.g., apparent resistivity, seismic travel-times, hydraulic head, and breakthrough times of tracer). Strictly speaking, measurements of system properties in hydrogeological site-characterization do not exist because these measurements are typically obtained by measuring other state variables from which an estimate is derived using a relationship that is valid under certain conditions (e.g., Butler, 2005). Rather, measurements of system properties denote estimates that have been made outside our estimation procedure and we must assume that they are known to a certain degree of accuracy.

1.2.1 Project objectives and available data

The need for information about the structure of hydrogeological properties occurs in many applications and at many different scales. The objectives, site characteristics, and available geophysical and hydrogeological data vary on a case-by-case basis, and attempts to estimate hydrogeological properties using geophysical data must take these characteristics into account. In this chapter, we consider these characteristics as given (e.g., we do not consider experimental design). Instead, we attempt to provide some guidance on how to formulate a hydrogeophysical parameter estimation method that matches specific objectives and provides a level of detail that can be resolved given the available data. In practice, other factors related to available budget, expertise, and computational facilities will be influential in determining the approach taken.

1.2.2 Model parameterization

Model parameterization depends on the research objectives and the available data. Regularization is a necessary step towards defining a well-posed inverse problem (e.g., Tikhonov and Arsenin, 1977). We must find ways to constrain model space in order to obtain meaningful results. We consider three approaches to model parameterization: zonation (e.g., Carrerra and Neuman, 1986a, b, c); geostatistical (e.g., Hoeksema and Kitanidis, 1984; Dagan, 1985); and Tikhonov regularization approaches (e.g., Tikhonov and Arsenin, 1977; Constable et al., 1987).

Zonation is used in applications where we assume that the earth can be divided into a number of zones where the variations of a property within the zones are small compared with the variations between the zones. Possible applications where a zonation approach could be justified are the delineation of sand from interbedded clay layers or sediments from the underlying bedrock. The advantage of the zonation approach is that the number of model parameters can be relatively small and smoothness constraints in the inversion may thus be avoided. Auken and Christensen (2004) demonstrated that this approach is preferable when mapping large-scale hydrogeological units in sedimentary environments using electrical methods. Such an approach also allows straightforward incorporation of measurements of system properties derived from borehole logs (Auken and Christensen, 2004). The zonation approach is probably the best approach when geological structure is apparent and formation boundaries are distinct (McLaughlin and Townley, 1996). However, the influence of the model parameterization is strong in zonation approaches and it might be difficult to reach conclusive results (e.g., Constable et al., 1987). Hydrogeological inversion codes that fall into this category are non-linear regression models such as the freely available UCODE (Hill, 1992) and MODFLOWP (Poeter and Hill, 1998), where regularization is imposed through model parameterization and/or by keeping certain model parameters fixed.

The geostatistical parameterization assumes that the parameter of interest is a spatial random variable with a certain correlation structure and sometimes a deterministic trend (e.g., Gómez-Hernández, 2005). This correlation structure typically includes a variance and integral scales that might vary in different directions (i.e., anisotropy). The geostatistical approach thereby decreases the number of effective parameters through spatial correlations and a known variance. A geostatistical parameterization is probably preferable when parameters vary in more or less random fashion and there is no clearly defined structure (McLaughlin and Townley, 1996).

The dominant approach to geophysical inversion is a fine grid discretization, where regularization is achieved through smoothing (i.e., finding the model that fits the data with minimum structure), damping (i.e., finding the model that fits the data and is the closest to an initial model) or a combination of smoothing and damping (Tikhonov and Arsenin, 1977; Maurer et al., 1998). Maurer et al. (1998) showed that a known mean and spatial correlation structure of a system property can be described by a combination of smoothing and damping; thereby, indicating a strong similarity between Tikhonov regularization approaches and geostatistics. However, the perspective is quite different. Tikhonov regularization is imposed to find a unique model (i.e., to make an ill-posed inverse problem well-posed). However, in geostatistical formulations the model covariance structure is honoured because it is assumed to describe real characteristics of the site. Damping has recently also been introduced in geostatistics (Kitanidis, 1999).

Our brief discussion on model parameterization shows that some understanding of the site characteristics is helpful in determining an appropriate model parameterization (e.g., Auken and Christensen, 2004). From this we can infer that resulting parameter estimates are not just determined by the data, but also by seemingly innocent choices of model parameterization and regularization.

1.2.3 The petrophysical relationship

How are geophysical and hydrogeological properties related? This is one of the most difficult questions in the efforts of hydrogeophysical parameter estimation. We should strive to choose a representation of the petrophysical relationship that reflects our understanding. This leads us to consider petrophysical relationships that are either:

- physically or empirically based;
- intrinsic or model-based;
- parameterizable or non-parameterizable;
- unique or non-unique; and
- stationary or non-stationary.

Below we briefly describe these petrophysical relationship characteristics. Since it is not within the scope of this chapter to provide detailed descriptions of physically based and empirical petrophysical relationships and the reader is referred to reviews given by Mavko et al. (1998), Lesmes and Friedman (2005), and references therein.

1.2.3.1 Physically or empirically based petrophysical relationship

Let us consider the problem of inferring water saturation in the vadose zone using radar data. In low loss material and for radar frequencies the EM wave velocity v (m/s) is related to the dielectric constant through (Davis and Annan, 1989):

$$v \approx \frac{\mathrm{c}}{\sqrt{\kappa}}, \tag{1}$$

where c is the EM wave velocity in free space (3×10^8 m/s) and κ is the effective dielectric constant. An approximate value of the effective dielectric constant can be calculated using the so-called complex resistive index method (CRIM) (Tinga et al., 1973; Alharthi and Lange, 1987; Roth et al., 1990):

$$\kappa = \left[(1-\varphi)\sqrt{\kappa_s} + S_w\varphi\sqrt{\kappa_w} + (1-S_w)\varphi\sqrt{\kappa_a}\right]^2, \tag{2}$$

where φ is porosity, S_w is water saturation, κ_s, κ_w, and κ_a are the dielectric constants for the solid, water, and air components of the soil, respectively. By combining equations (1)-(2) we can estimate the water saturation if we have an estimate of porosity, radar velocity, and the permittivity of the earth material:

$$S_w = \frac{\left(\frac{c}{v} + (\varphi - 1)\sqrt{\kappa_s} - \varphi\sqrt{\kappa_a}\right)}{\varphi\left(\sqrt{\kappa_w} - \sqrt{\kappa_a}\right)}. \tag{3}$$

Using a physically based approach, it is straightforward to relate uncertainties in model parameters with uncertainties in the resulting estimate. As an example, we show confidence limits for the case where it is assumed that κ_s, φ, and υ are normally distributed, where κ_s has a mean of 4 and a standard deviation of 1, φ has a mean of 0.35 and a standard deviation of 0.02, and that υ has a standard deviation of 1 m/μs (Figure 1). We see that substantial prediction errors in the estimation of saturation occur, even when parameters are well-defined and the structure of the petrophysical model is assumed to be known. For this example, the dominating cause of uncertainty is the uncertainty of κ_s.

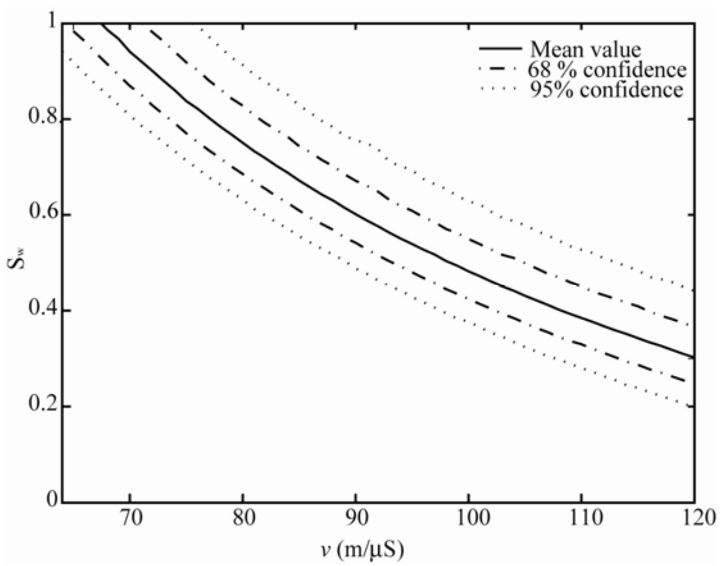

Figure 1. A petrophysical model between radar velocity, υ, and water saturation, S_w, based on the CRIM model. The resulting confidence intervals are shown assuming normally distributed random errors in the radar velocity, porosity, and the effective dielectric constant of the solid.

Most often, we rely on semi-empirical relationships (such as Archie's law; Archie, 1942) or purely empirical relationships (such as a linear regression between log electrical conductivity and log permeability measurements; Purvance and Andricevic, 2000a). These relationships are much more difficult to work with because (1) we need to estimate a site-specific relationship and (2) we have limited understanding of the validity of this relationship away from the calibration points. However, this is often the only possibility and several successful case studies are given in the literature (e.g., Purvance and Andricevic, 2000b; Hubbard et al., 2001).

1.2.3.2 Intrinsic or model-based petrophysical relationship

We define the intrinsic petrophysical relationship as the relationship between the true geophysical and hydrogeological properties; and we define the model based petrophysical relationship as the relationship between our geophysical and hydrogeological model parameters. The intrinsic relationship is unknown to us. Laboratory analysis might provide a good estimate, although it may be difficult to scale the relationship for use at the field scale (e.g., Moysey and Knight, 2004). Day-Lewis and Lane (2004) compared the correlation between a synthetic slowness (i.e., the inverse of velocity) structure and the estimated slowness structure derived from a hypothetical radar survey. They showed that the linear correlation factors between these two structures were space-varying, significantly less than one, a function of acquisition errors, survey geometry, and regularization. This implies that the model based petrophysical relationship is different from the intrinsic petrophysical relationship and that it might be non-stationary even if the intrinsic petrophysical relationship is stationary. This is problematic, because:

- if we use a physically based relationship, such as (3), or a close approximation of the intrinsic relationship based on laboratory analysis, its predictive power will be significantly decreased if we use it to relate our estimated geophysical model with hydrogeological properties and it might give biased results;
- an empirical relationship estimated by regression of collocated hydrogeological data and estimated geophysical parameters will not be strictly valid throughout the model domain even if all properties except the geophysical and hydrogeological parameters of interest are kept constant; and
- relationships that we establish in the field are not only a function of hydrogeological characteristics, but also of acquisition errors, survey geometry, and regularization of the inverse problem. These campaign-related errors reduce the validity of the developed relationships for use at other sites.

How large are these potential errors compared with other error sources and with regard to the accuracy needed to meet specific model objectives? It is not always necessary to have very detailed estimates and the effects discussed above might be insignificant in certain applications, such as mapping of the interface between salt and freshwater in coastal aquifers where the formation factor is determined using borehole information and applied to large scale resistivity models. However, these effects are probably significant if we attempt to provide high-resolution characterization at the local scale in order to predict solute transport.

1.2.3.3 Weak or no parameterization of the petrophysical relationship

In some cases, a relationship between a geophysical and a hydrogeological parameter may not exist or it may be very weak. For example, Pride (2005) stated that there is no theoretical basis for a universal relationship between seismic velocity and permeability in porous media. However, site specific models may exist (Pride, 2005; Hubbard et al., 2001; Hyndman et al., 2000), although they may vary within short distances (Prasad, 2003). It has been argued that the logarithm of electrical conductivity and the logarithm of permeability have a linear relationship, but the slope is site-specific and it is very sensitive to clay content (Purvance and Andricevic, 2000a).

In cases where the petrophysical relationships are weak, zonation approaches (see section 1.2.2) can potentially be useful to quantify the geometry of hydrofacies. Borehole information and tracer test data can subsequently be used to estimate the hydrogeological properties of these zones (e.g., Hyndman et al., 1994; Hyndman and Gorelick, 1996; McKenna and Poeter, 1995, see also section 1.5.1). Such an approach is useful when different facies have distinctly different geophysical properties because under such circumstances the determination of facies becomes relatively insensitive to errors in the geophysical data acquisition and the subsequent inversion. Alternatively, if we use a geostatistical parameterization or an Occam type of inversion we could impose restrictions on the model space. An example is provided by Gallardo and Meju (2004) who jointly inverted seismic refraction data and surface dc resistivity data by restricting the model space of the two models to models where the cross-gradients, $\boldsymbol{t}$, of the models were zero. The cross-gradient in the case of one geophysical model, $\boldsymbol{m}_g$, and one hydrogeological model, $\boldsymbol{m}_h$, is defined as

$$\boldsymbol{t}=\nabla\boldsymbol{m}_g\times\nabla\boldsymbol{m}_h. \quad (4)$$

This approach has yet not been incorporated in hydrogeophysics, but it is promising because structural similarity between models is emphasized instead of a petrophysical relationship that is difficult to justify in many applications.

In short, the representation of the petrophysical relationship is one of the most difficult tasks in hydrogeophysical parameter estimation. A precautionary attitude is recommended.

1.2.4 A-priori information

A-priori information is information about characteristics of the models that we get from other sources of information rather than the actual geophysical or hydrogeological data. Prior information in deterministic inversions is used to define bounds of possible models, such as ensuring that velocities are positive, or assuming that the electrical resistivities are below 10 000 ohm-m in a sedimentary basin. These bounds should ideally represent information that is known without doubt. Stochastic inversion theory takes an additional step by assigning a probability distribution of the possible model parameters before any measurements are made (e.g., Tarantola, 1987).

A-priori information is sometimes used to tune the model to get agreeable features of the solution or make it well-posed. This violates a pure use of a-priori information, but might be a good place to incorporate subjectivity, if needed. We agree with the ironic comment made by Jackson (1979) in discussing the use of a-priori information to resolve non-uniqueness: "One disadvantage of the technique is that the assumptions which lie hidden in the abstractness of most methods are in this method left naked for the world to see". An excellent tutorial to the use of a-priori information is Scales and Tenorio (2001), and Malinverno and Briggs (2004) provided a discussion on how hierarchical and empirical Bayes can be used to avoid assuming that the probability distribution function is known.

1.2.5 Optimization or Monte Carlo methods

Local optimization methods are the most common parameter estimation approaches and model uncertainties are typically evaluated around the solutions that minimize the objective function. Uncertainty is thus often described in terms of a standard deviation of the model parameters or through sensitivity analysis of what parameters are better determined than others. Furthermore, in a deterministic approach only uncertainties in the data are assumed. Uncertainty estimates performed in this way are often over-optimistic. Another form of uncertainty arises if the problem is strongly non-linear because it might result in local minima. There are ways to decrease non-linearity, such as transformation of the data, weighting, and alternative parameterizations of the models. We can also assess the existence of local minima by trying different initial and prior models (e.g., Oldenburg and Li, 1999). Even if we find the global minimum it does not mean that we can disregard other local minima. An alternative is to carry out a global search to derive the posterior pdf of all model parameters. Markov chain Monte Carlo Methods (MCMC) are often performed for computational efficiency using the Metropolis-Hastings algorithm (e.g., Mosegaard and Tarantola, 1995) or Gibb's sampling (e.g., Chen et al., 2003), as will be described in sections 1.4.3 and 1.5.3.

1.2.6 Objective functions

In this section, we discuss common objective functions used in different estimation procedures. The treatment is cursory and it is mainly given to illustrate in a simple fashion how different methods are interconnected and to provide relevant references. We also spend some time discussing Occam's inversion because of its widespread use in geophysical inversion. Geophysical inverse theory is treated by Menke (1984), Parker (1994), and Tarantola (1987); an excellent review of hydrogeological inversion is given by McLaughlin and Townley (1996). A formalized treatment of stochastic forward and inverse modeling in hydrogeophysics is given by Rubin and Hubbard (2005).

The data fit χ_d^2 is often defined as

$$\chi_d^2 = (\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])^{\mathrm{T}} \mathbf{C}_{\mathbf{d}}^{-1} (\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}]), \tag{5}$$

where $\boldsymbol{d}$ is an N×1 data vector (e.g., seismic travel times, mass fractions of tracer); $\mathbf{F}$ is a forward model operator; $\mathbf{C}_{\mathbf{d}}^{-1}$ is the inverse of the data covariance matrix. It is commonly assumed that $\boldsymbol{d}$ is uncorrelated, rendering the $\mathbf{C}_{\mathbf{d}}^{-1}$ a diagonal matrix that contains the inverses of the estimated variances of the observation errors; thus, more reliable data carry larger weight. Our data covariance matrix can either be estimated or assumed to take certain values if the method does not allow an error estimate. There is an implicit assumption of Gaussian errors in this formulation of the data fit. This is neither the only nor necessarily the best description of data fit, but it is without doubt the most commonly used. Huber (2003) provides a review of robust statistics and Finsterle and Najita (1998) discuss robust estimation in hydrogeology.

A general description of the model norm assuming that the model parameters have a Gaussian distribution is

$$\chi_m^2 = (\boldsymbol{m} - \boldsymbol{m_0})^{\mathrm{T}} \mathbf{C}_{\mathbf{m}}^{\mathbf{-1}} (\boldsymbol{m} - \boldsymbol{m_0}), \tag{6}$$

where $\boldsymbol{m_0}$ is an a-priori model of size M×1; and $\mathbf{C}_{\mathbf{m}}^{\mathbf{-1}}$ is the inverse of the model covariance matrix, which characterizes the expected variability and correlation of model parameters. However, the model covariance matrix is often unknown and it might be restrictive to damp the model to be close to an initial model, if no good initial model exists. Therefore, other model norms are typically defined using different measures of roughness (Constable et al., 1987), e.g., based on the first derivatives of the model

$$\mathrm{R}_1 = (\partial \boldsymbol{m})^{\mathrm{T}} (\partial \boldsymbol{m}), \tag{7}$$

where ∂ is an N×N matrix given by

$$\partial = \begin{bmatrix} 0 & & & \\ -1 & 1 & & 0 \\ & \dots & \dots & \\ & 0 & -1 & 1 \end{bmatrix}. \tag{8}$$

The data fit and measures of model structure can be combined to formulate the most common objective functions.

A weighted least-squares objective function (equation 5) is used when we do not have any a-priori information and when the inverse problem is well-posed without adding a regularization term. However, this is typically not the case and we must impose a-priori information, justified or not. The corresponding objective function corresponds with the maximum a-posteriori (MAP) estimate (e.g., Menke, 1984):

$$\phi_{MAP} = (\boldsymbol{m} - \boldsymbol{m_0})^{\mathrm{T}} \mathbf{C}_{\mathbf{m}}^{\mathbf{-1}} (\boldsymbol{m} - \boldsymbol{m_0}) + (\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])^{\mathrm{T}} \mathbf{C}_{\mathbf{d}}^{\mathbf{-1}} (\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}]). \tag{9}$$

This is a weighting of a-priori assumptions and data. However, we do not always have a good estimate of the model covariance and the data errors. Furthermore, the inverse problem may still not have a unique solution (e.g., the integral scales are extremely short). This is the reason why Occam types of inversion are so popular in geophysical applications. We briefly review Occam's inversion (Constable et al., 1987), which was originally developed for plane-wave electromagnetic data, but has been applied to diverse problems, including resistivity tomography (e.g., the commercial software Res2DInv of Loke (1997)). The goal of Occam inversion is to minimize R_1

(or any other measure of model roughness) subject to $\chi_d^2 = \chi_*^2$, where χ_*^2 is the desired level of data misfit. We solve the problem by minimizing the penalty functional $W_\lambda(\boldsymbol{m})$

$$W_\lambda(\boldsymbol{m}) = (\partial\boldsymbol{m})^T(\partial\boldsymbol{m}) + \lambda^{-1}\left\{(\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])^T \boldsymbol{C}_d^{-1}(\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])\right\}, \qquad (10)$$

where λ^{-1} acts as a trade-off parameter between the smooth well-conditioned problem defined by a heavy penalty of model roughness (i.e., λ is large) and the ill-conditioned problem defined by the data fit (i.e., λ is small). For each iteration a line search for the λ that minimize χ_d^2 if $\chi_d^2 > \chi_*^2$, or else for the maximum λ for which $\chi_d^2 \le \chi_*^2$ is made.

Occam approaches fit the data to the level of the estimated data errors with the smoothest possible model. Thus, we must be careful in adopting Occam types of inversion in environmental applications. Occam's inversion was developed for interpretation of magnetotelluric data, which is a technique that provides actual data error estimates and where we, due to the large depth of investigation, often have very limited a-priori information. Therefore, it is sensible to be as conservative as possible. However, this method provides only a single model that might have little useful relations to the earth that gave rise to the observed data (Ellis and Oldenburg, 1994) and our prior knowledge. For example, it might be of little value to try to infer the spatial correlation structure of the model property from an Occam inversion. In short, Occam's inversion invariably provides models that are smoother than the true structure. Ellis and Oldenburg (1994) argue that we should construct alternative approaches that emphasizes the prior information and includes the observed data as a supplementary constraint. Please note that any a-priori model or model covariance matrix in principle could be included in the Occam formulation if the objective function to minimize is defined as (Siripunvaraporn and Egbert, 2000)

$$W_\lambda(\boldsymbol{m}) = (\boldsymbol{m} - \boldsymbol{m_0})^T \mathbf{C}_\mathbf{m}^{-1}(\boldsymbol{m} - \boldsymbol{m_0}) + \lambda^{-1}\left\{(\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])^T \mathbf{C}_\mathbf{d}^{-1}(\boldsymbol{d} - \mathbf{F}[\boldsymbol{m}])\right\}, \qquad (11)$$

which is identical to the MAP estimate (equation 9) if $\chi_d^2 = \chi_*^2$ is reached for λ=1.

1.2.7 Direct mapping, integration methods, or joint inversion methods

We divide hydrogeophysical parameter estimation approaches into three broad categories: (1) direct mapping; (2) integration methods; and (3) joint inversion methods. We define *direct mapping* as a transformation of a geophysical model into a hydrogeological model, where hydrogeological data are only used to develop a petrophysical relationship or provide a qualitative understanding of the relationship between the geophysical and hydrogeological property of interest. Direct mapping is discussed in Section 1.3. *Integration methods* refer to cases where the geophysical inversion is performed independently of hydrogeological data, and vice versa. The task is to interpolate available data or inverse models given their uncertainties, petrophysical relationships, and a-priori information. This group includes well-known geostatistical approaches such as co-kriging and Bayesian formulations; they are discussed in Section 1.4. Finally, *joint inversion methods* refer to cases where geophysical or hydrogeological inversion also utilizes hydrogeological or geophysical data, respectively. This diverse group is discussed in Section 1.5. There are large differences within each category and significant overlaps may exist in many published studies (e.g., McKenna and Poeter, 1995; Hyndman and Gorelick, 1996). The critical choices discussed in Section 1.2 must be made regardless of our choice between direct mapping, integration methods and joint inversion methods. These choices are of fundamental importance and an attempt to provide some guidance was made in Section 1.2.

Relying on a set of case studies, we now discuss the strengths and limitations of these three different categories of hydrogeophysical parameter estimation methods. The categories refer to the stage in which hydrogeological and geophysical properties are related. There are advantages in inferring this relation at an early stage, but it comes at a price, as is discussed in the following sections. Our primary focus is on joint inversion methods, because interesting developments are taking place in this area and they are much less reviewed than direct mapping and integration methods in the hydrogeophysical literature.

The following discussion focuses only on applications within hydrogeophysics. We do not review the the vast literature on data integration and joint inversion in other fields, such as in the petroleum (e.g., Deutsch, 2002) and mining engineering (e.g., Journel and Kyriakis, 2004) fields.

1.3 Direct mapping

The simplest approach to hydrogeophysical parameter estimation is to transform the geophysical model into an estimate of hydrogeological structure using a petrophysical relationship. This is the only possibility if we do not have any hydrogeological data. Hydrogeological data are absent or scarce in many applications, e.g., if we want to map a fracture zone for a potential well in sub-Saharan Africa (e.g., Caruthers and Smith, 1992); if we want to make preliminary investigations to find a site that meets our research objectives (e.g., Hubbard et al., 2001); or map salt-water intrusion (e.g., Yang et al., 1999). Such examples probably make up most applications in environmental geophysics. In such cases, it is important to use all available information and geological understanding to define the best possible geophysical model; ideally performing joint inversion of different geophysical data sets (e.g., Meju, 1996; Gallardo and Meju, 2004). However, it is generally not advisable to transform a geophysical estimate into a hydrogeological estimate if a petrophysical relationship with reasonably high predictive power is not available. It is often better to acknowledge our ignorance about the relation between our geophysical model and the underlying hydrogeological system and instead give qualitative interpretations, such as locations of possible clay lenses or fracture zones. Quantitative models could potentially be developed at a later stage when hydrogeological data become available. However, there are cases where direct mapping can be used for high-resolution studies of hydrogeological parameters. Water content estimation using Ground Penetrating Radar (GPR) is one example where direct mapping is often acceptable, and it is discussed in the next section.

1.3.1 Example 1: Estimation of water content

In recent years, GPR has developed as a tool for mapping water content and movement within the vadose zone. A review of GPR concepts and applications in hydrogeological applications is provided by Annan (2005).

As recently summarized by Huisman et al. (2003), a variety of GPR approaches have been successfully used to estimate soil water content, including the use of ground-based GPR ground-wave and reflection data, and GPR crosshole tomographic direct wave travel time data. With most approaches, the velocity is first estimated and is then converted to a dielectric constant using equation (1), which is then converted to water content using relationships such as equation (3). For example, Grote et al. (2003) used the GPR ground-wave travel time data to estimate volumetric water content, and reported a volumetric water content RMS error of 0.011 to 0.017 using 900 and 450 MHz antennas, respectively. Fisher (1992), Greaves et al., (1996), and van Overmeeren et al. (1997) used common midpoint (CMP) approaches to estimate water content. In general, the time required to collect CMP data makes this approach prohibitive for water content estimation over large areas, and the error associated with CMP velocity analysis is typically on the order of 10% (Tillard and Dubois, 1995, Greaves et al., 1996). Common-offset GPR data are faster and easier to collect, although in order to estimate the velocity of the reflected wave, one must have information about the depth of the reflector. Grote et al. (2002) investigated the utility of the GPR common-offset approach using reflectors buried at a known depth, and found that this approach was accurate to within 0.01. More recently, Lunt et al. (2005) used wellbore information together with common offset GPR reflection data to assess the error associated with the GPR water content reflection method under natural conditions. Lunt et al. (2005) found that the RMS water content error under natural conditions was 0.018. Hubbard et al. (2005) used the GPR reflection travel time data of Lunt et al. (2005), together with wellbore soil layer depth information within a Bayesian framework to estimate water content associated with an interface located 0.5-1.4 m below ground surface over a 2.5 acre field site.

Crosshole radar methods are now used quite frequently to map or monitor water content (Hubbard et al., 1997; Binley et al., 2001; Peterson, 2001; Alumbaugh et al., 2002). For tomographic acquisition, the transmitter and receiver position are varied until the entire interwell area is traversed by electromagnetic waves. Inversion algorithms are used to invert the GPR travel time data into velocity (e.g., Peterson, 2001), which are then translated into dielectric constant using equation (1) and water content estimates using relations such as equation (3). It should be noted that ray-based tomographic techniques invert for slowness (i.e., the inverse of velocity). Alumbaugh et al. (2002) showed that water content estimates obtained from crosshole GPR have an RMS error of 0.03. Crosshole surveys are useful in that they can provide high-resolution two-dimensional images of water content at one point in time, or, when measured in a time-lapse sense, as a function of time (Hubbard et al., 1997; Eppstein and Dougherty, 1998; Binley et al., 2002; Day-Lewis et al., 2003). Although crosshole tomographic radar data are becoming more commonly used for moisture monitoring, the maximum borehole separation distance of about 15 m generally limits this technique to very local-scale investigations.

An example of the use of crosshole radar data for estimating volumetric water content is illustrated using data collected within the porous granular vadose zone of the DOE Hanford Site in Washington (Ward et al., 2000; Gee and Ward, 2001). Neutron probe data were collected at this site, calibrated using gravimetric techniques, and interpreted in terms of volumetric water content (Ward et al., 2000). Tomographic GPR data were collected using the PulseEKKO 100 GPR system and 200 MHz antennas (Majer et al., 2000). Inversion of the tomographic travel time data was performed following Peterson (2001), and used with (1) to estimate dielectric constants. Equation (3) was used to convert the dielectric constant estimates to water content, with κ_s=5.6 (Kowalsky, 2004b), and φ=0.345 (inferred from saturated water content values of Zhang et al. (2004)). Figure 2a shows the 2-D distribution of estimated volumetric water content between two wells, and Figure 2b shows a comparison of neutron probe values collected from an access tube located close to X3 with the estimates of water content obtained from the tomographic pixels along the column located approximately 0.25 m away from X3 wellbore (to avoid the geophysical distortion commonly encountered at the wellbore location). This figure illustrates that a simple mixing model was sufficient for estimating water content in multiple directions with a reasonable accuracy, and thus highlights the use of GPR for direct mapping of water content.

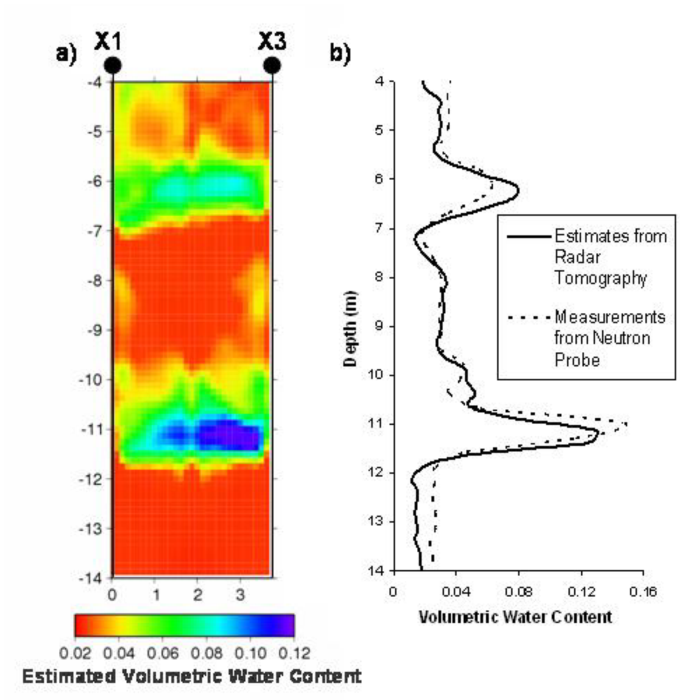

Figure 2. (a) Volumetric water content estimated using tomographic radar data, (b) comparison of tomographic estimates and neutron probe measurements of water content near borehole X3.

1.4 Integration methods

By integration methods, we refer to approaches where the geophysical inversion is carried out independently of the hydrogeological data or where the hydrogeological inversion is carried out independently of the geophysical data. Integration methods are widely used and we discuss two types: co-kriging and Bayesian approaches.

1.4.1 Co-kriging

Co-kriging (Deutsch and Journel, 1992) is a widely used method in geostatistics; it is essentially kriging conditioned on secondary information. Co-kriging is valid if we can represent the data such that measurement errors are Gaussian with a known variance; the area under study is stationary or stationary within large areas; and if the relation between the attributes is linear and known. The estimate is an expected mean behavior and it should not be considered as a realistic model estimate of the true system properties. A classical application of co-kriging is to infer the transmissivity distribution of an aquifer using transmissivity estimates and hydraulic head data (e.g., Clifton and Neuman, 1982). Applications of co-kriging using hydrogeological and geophysical data include Doyen (1988), Pesti et al. (1993), Parks and Bentley (1996), Cassiani and Medina (1997), Lesch et al., (1995), Cassiani et al., (1998), and Gloaguen et al., (2001).

Co-kriging is a straightforward method to apply and it is useful when the assumptions behind the method are valid and the type of information obtained is sufficient for project objectives. Drawbacks with the method are that the estimation variance only gives a qualitative estimate of model uncertainty and the estimated model is unrealistically smooth.

1.4.2 Bayesian methods

Bayes' theorem is an appealing framework for integration of different types of data and a-priori information. General literature on Bayesian methods includes Press (1989) and Sivia (1996).

A Bayesian formulation of data integration is more general than co-kriging because it allows any prior distribution as well as non-linear likelihood functions. Chen et al. (2001) combined collocated geophysical estimates of GPR velocity, GPR attenuation, and seismic velocity with permeability estimates from flowmeter data to estimate the likelihood functions for the case of three geophysical data types. The likelihood function was estimated through a normal linear regression method. The prior was a kriged estimate of the permeability structure where the correlation structure has been estimated using available geophysical models and permeability data. This approach was used to estimate the permeability structure at the South Oyster Bacterial Transport Site (Chen et al., 2001; Hubbard et al., 2001).

In the next section, we will give an example of an integration method for geochemical characterization.

1.4.3 Example 2: Geochemical characterization

Traditional methods for characterizing geochemical heterogeneity typically involve drilling a borehole and either retrieving a soil sample for laboratory analysis or collecting borehole logs within the hole. Although these methods are deemed necessary for collecting data to understand field-scale bacterial transport processes, it is prohibitive to use them intensively for collecting dense data to estimate geochemical parameters in a multi-dimensional domain. Borehole-sampling methods combined with geophysical methods, hold potential for improved geochemical characterization, as is discussed below.

This study demonstrates the use of GPR tomographic data collected at the DOE South Oyster Bacterial Transport Site in Virginia for estimating solid-phase Fe(II) and Fe(III) concentrations using a sampling-based Bayesian model. By exploiting the site-specific mutual dependence of GPR attenuation and extractable Fe(II) and Fe(III) concentrations on lithofacies (developed using co-located GPR attenuation pixel values and soil sample measurements), a Bayesian model was developed. Within the model, lithofacies and Fe(II) and Fe(III) concentrations at each pixel between the boreholes were considered as random variables. The borehole lithofacies measurements and crosshole GPR tomograms (Figure 3a) were considered as independent parameters. By conditioning all the unknowns to the available datasets, a joint posterior probability distribution function of those variables was defined at each location. Using a Markov chain Monte Carlo (MCMC) method, many samples of each unknown were obtained, which were subsequently used to calculate mean, variance, and predictive intervals for each unknown variable.

Cross validation was performed based on data at the three wells, shown as wells D1, D2, and D3 in Figure 3, to assess the accuracy of the developed estimation method. Each well in turn was considered as a testing well and the other two wells as training wells. Cross validation results show that the geophysical data, constrained by lithofacies, have the potential for providing high-resolution, multi-dimensional information on extractable Fe(II) and Fe(III) concentrations at the South Oyster site.

Figures 3(b)-(d) show the two dimensional images of the estimated mean logarithmic extractable Fe(II) concentrations, the probability of sand lithofacies, and the mean logarithmic extractable Fe(III) concentrations, respectively. It is evident that with the help of high-resolution GPR tomograms, the measurements of extractable Fe(II) and Fe(III) as well as lithofacies measurements can be extended to locations where direct measurements are not available. For details, see Chen et al. (2004).

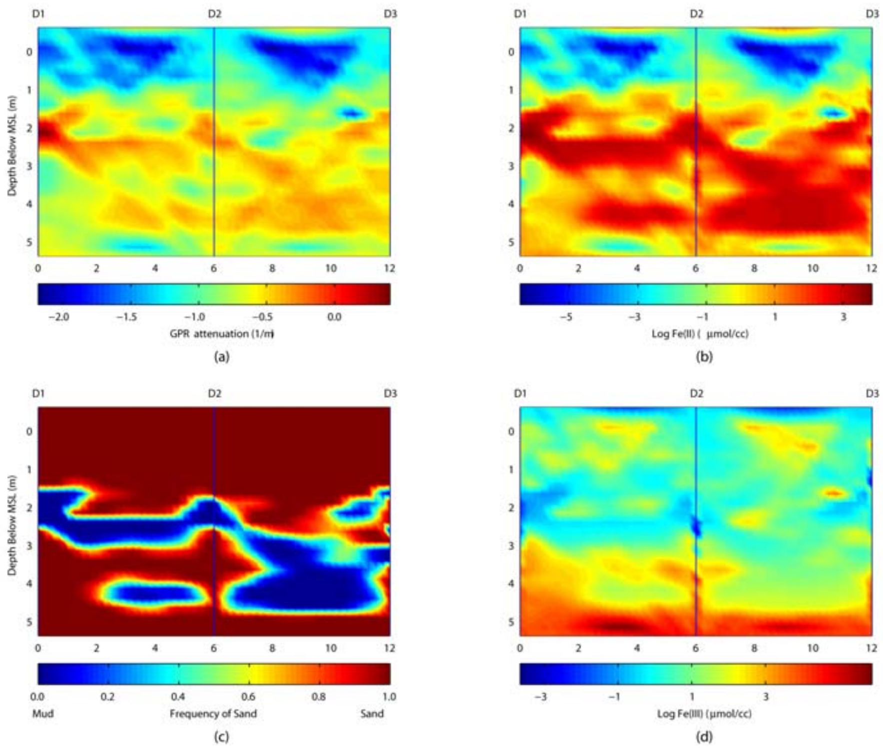

Figure 3. (a) GPR attenuation; (b) estimated mean natural logarithmic Fe(II) concentrations; (c) frequency of sand (a frequency of 0.0 implies that lithofacies is mud, whereas a frequency of 1.0 implies that lithofacies is sand); (d) estimated mean natural logarithmic Fe(III) concentrations (from Chen et al., 2004).

1.4.4 Discussion of integration methods

Integration methods are relatively easy to implement because geophysical inversion and hydrogeological data processing are carried out separately. Furthermore, they rely on well-established techniques to integrate different types of data. This category of parameter estimation methods is relatively mature, and many successful case-histories exist (e.g., Cassiani and Medina, 1997; Chen et al., 2001; Hubbard et al., 2001; Chen and Rubin, 2003; Chen et al., 2004). However, they have some inherent limitations.

- The geophysical inverse models used in the estimation could potentially be improved if we incorporate hydrogeological data in the geophysical inverse procedure because of information sharing. Integration methods do not take advantage of this opportunity.

- Geophysical models typically have a spatially varying resolution. We should strive to constrain our hydrogeological models to the features that are well constrained in the geophysical inversion, and avoid interpreting phantom structures or features that are not related to hydrogeological properties. In principle, it may be possible to assign different weights to areas with different resolution. In practice, however, it is difficult to estimate those weights. This is a common problem in the interpretation of any geophysical model. One way to decrease the effects of this problem is to incorporate the geophysical inversion (Hyndman et al., 1994; Hyndman and Gorelick, 1996) or the geophysical model (Hyndman et al., 2000; Linde et al., 2004) as a part of the hydrogeological inversion (see section 1.6.1).
- We often assume that the petrophysical relationship is stationary and use it over the entire spatial domain. In practice, non-stationary petrophysical relationships are common. For example, we know that intrinsic petrophysical relationships might show non-stationary behavior under certain conditions (e.g., Prasad, 2003; Yeh et al., 2002). Even a perfect stationary intrinsic relationship may break down in the geophysical inversion (Day-Lewis and Lane, 2004). More discussion of stationarity was provided in section 1.2.2.
- How should we estimate the model based petrophysical relationships? The natural choice is to compare collocated tomographic pixels and nearby borehole information (e.g., Chen et al., 2001; Hubbard et al., 2001). However, for ray-based tomography (GPR and seismic), the resolution of the inverted geophysical data at or near boreholes is worse than the resolution in the central parts of the tomograms (e.g., Day-Lewis and Lane, 2004), whereas the resolution is best close to the borehole in ERT applications. Thus, the location where co-located data are used to develop a site-specific relationship can impact its accuracy. In addition, the environment around the boreholes may be disturbed by the drilling, altering both the hydrogeological and the geophysical measurements and thus further complicating the task of estimating a valid petrophysical relationship throughout the tomogram.
- In integration methods, we often assume that the resolution of the geophysical models is fine enough that the resulting hydrogeological parameter estimates can capture all important variations of hydrogeological parameters. This assumption might not be valid in

some applications because we know that the tomograms are smooth estimates of the true geophysical structure and that they have a limited resolution (e.g., Day-Lewis and Lane, 2004).

Moysey et al. (2005) presented a methodology to address some of the limitations associated with the development of petrophysical relationships. In their study, a stochastic calibration method was developed to estimate field-scale estimates of petrophysical relationships given a petrophysical relationship at the core scale. The methodology enlarged existing well-log data by generating additional conditional realizations of the property of interest (e.g., water content) using petrophysical relationships and geostatistical information. These realizations were mapped into geophysical realizations (e.g., dielectric constant) using the appropriate petrophysical relationship at the core scale (e.g., the CRIM formula). Synthetic geophysical surveys were performed and inversions of these realizations were made. Using this approach, average or pixel-specific field-scale petrophysical relationship could be developed that takes scaling, measurement errors, uncertainties in the petrophysical relationship, and the inversion process into account. Moysey et al. (2005) illustrated for a synthetic example how the methodology improved water content estimation using radar tomograms compared with the case where the underlying core scale relationship was applied to map the tomographic estimate into water content. However, in addition to borehole logs, reasonable knowledge is needed about the spatial correlation of the property of interest, the errors of the data, and the petrophysical relationship at the core-scale. Nonetheless, the study indicates how the hydrogeophysical community has recognized some of the limitations involved in earlier estimation approaches and how efforts are underway to overcome these obstacles.

In the next section, we discuss how joint inversion methods can improve estimates compared with integration methods. However, the limitations listed above will always apply to some degree.

1.5 Joint inversion methods

In section 1.2.7, we gave the following definition: “by joint inversion methods we refer to cases where geophysical or hydrogeological inversion also utilizes hydrogeological or geophysical data, respectively”. Thus, joint inversion includes many different approaches for hydrogeophysical parameter estimation, including:

- geophysical inverse modeling that incorporates measurements of hydrogeological system properties;
- geophysical inverse modeling that incorporates both measurements of hydrogeological system properties and measurements of dependent hydrogeological variables;
- hydrogeological inversion that is regularized by geophysical models, and maybe also by measurements of hydrogeological system properties; or
- both hydrogeological and geophysical inverse modeling are conditioned to both measurements of hydrogeological and geophysical system properties, as well as dependent hydrogeological and geophysical variables. These joint inversion models can either be updated simultaneously or in a sequential fashion.

Joint inversion of hydrogeological and geophysical data sets is a current topic of research (e.g., Yeh et al., 2002). In the following, we present several examples in which joint inversion models were applied, including the zonation of a 3-D structure in a sandy aquifer (see section 1.5.1); estimation of flow parameters in the vadose zone (see section 1.5.2); and delineation of fracture zones (see section 1.5.3). Finally, we gather the experiences from these examples and other studies to make some concluding remarks on joint inversion methods.

1.5.1 Example 3: Zonation of permeability

Hyndman et al. (1994) performed coupled seismic and tracer test inversion in a 2-D synthetic aquifer in order to estimate zones of high and low permeability. The motivation for this study was that geophysical information might help in estimating the permeability structure, but that it is sometimes not justified to impose a known petrophysical relationship. The assumption behind their approach was that changes in lithology manifest as large changes in seismic velocity. Furthermore, they argued that groundwater flow is often predominantly controlled by large-scale heterogeneities. Their approach was based on a division of the seismic velocities into two classes. They applied their split inversion methodology (SIM), which essentially estimates a tomogram with zones delineating the spatial distribution of two lithological classes. The permeabilities of the classes were determined using tracer test data. The zonation was updated by minimizing the squared misfit of seismic travel times and tracer test data. The permeabilities within the classes were updated. This procedure was repeated in an iterative fashion.

Hyndman and Gorelick (1996) extended this analysis to 3-D and three unique lithological classes. They applied their method to the Kesterson aquifer. They observed a reasonably good data fit to the tracer test data. Hyndman et al. (2000) established a linear field scale model based petrophysical relationship between seismic velocity and permeability. They do this by transforming realizations of the seismic velocity structure at Kesterson into permeability. The relationship between seismic velocity and permeability has a correlation factor of 0.74, which can be compared with a relationship of 0.16 using borehole data. The tracer test data were better explained when the permeability realizations were performed using both hard permeability data and soft seismic slowness data (Figure 4b) compared with only permeability data (Figure 4a).

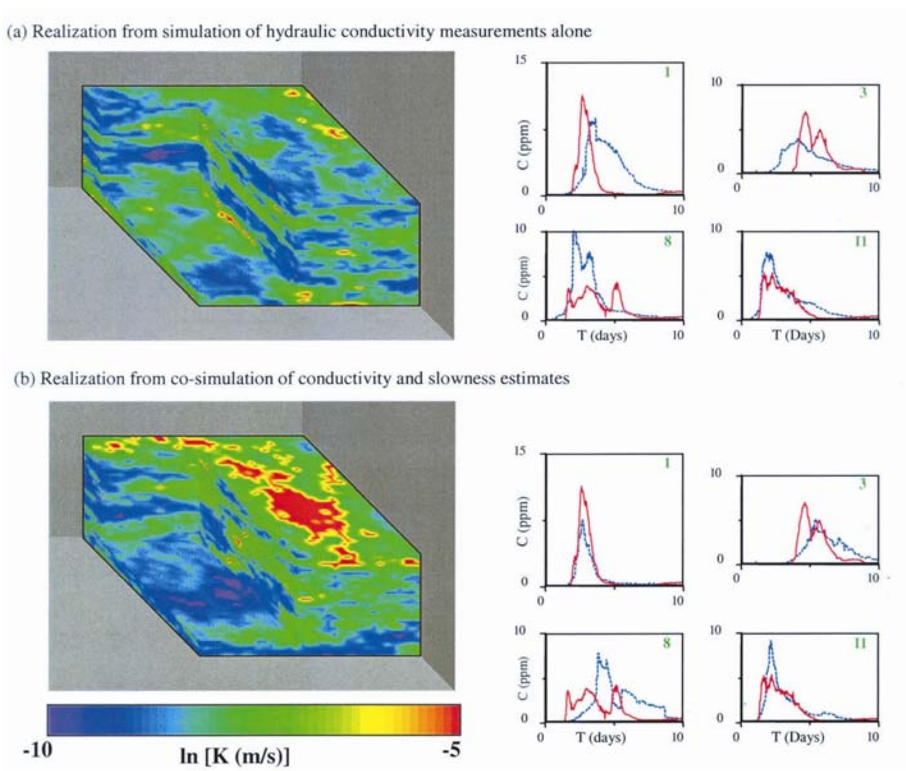

Figure 4. Comparison of tracer concentration histories for the 1986 fluorescein test at the Kesterson aquifer simulated through permeability realizations (a) generated using permeability measurements alone and (b) generated using sequential Gaussian cosimulation with hard permeability data and soft seismic slowness data from a seismic realization (adopted from Hyndman et al., 2000).

1.5.2 Example 4: Vadose zone parameter estimation using time-lapse GPR travel time data

Crosshole GPR measurements are being used increasingly for monitoring transient flow processes in the vadose zone, thanks to their high sensitivity to pore water distribution in the subsurface (see equation (2)). As described in Section 1.3.1, tomographic inversion techniques (e.g., Peterson et al., 2001) are typically applied to crosshole GPR data sets to infer spatial distributions of electromagnetic velocity or dielectric constant, which can be related to water saturation through a petrophysical relationship, such as equation (3). However, while tomographic techniques are useful for gaining a qualitative understanding of flow processes (such as identifying flow directions and preferential flow paths), in general they cannot be used to obtain quantitative estimates of vadose zone flow parameters, such as permeability and the soil hydraulic parameters of the capillary pressure and relative permeability functions.

In the present section, we describe an alternative approach for using crosshole GPR data that allows flow parameter distributions to be estimated in the vadose zone. This approach, described in detail by Kowalsky et al. (2004a), involves the joint inversion of hydrological and geophysical measurements collected during transient flow events. Geophysical observations are indirectly related to the hydraulic parameters: for any given soil hydraulic parameter estimates, a flow experiment is simulated and the resulting distributions of water saturation are used as input to simulate dependent geophysical variables. Inversion proceeds by perturbing the hydraulic parameters—which causes changes in the simulated water distributions and the subsequent dependent geophysical variables—until a good match between simulated and measured geophysical and hydrological data is achieved.

The example considered by Kowalsky et al. (2004a) involves the case where the only non-uniform flow parameter is the permeability, and it can be treated as a log normally distributed space random function (SRF) with known patterns of spatial correlation. Through a maximum a posteriori (MAP) inversion framework that employs concepts from the pilot point method, the log permeability distribution and additional flow parameters can be estimated. This methodology allows for the generation of multiple parameter distributions that reproduce measurements of permeability, that contain the specified patterns of spatial correlation, and that are consistent with the hydrological and geophysical data; these parameter distributions can be used for hydrological modeling and also to calculate parameter probability density functions, which provide a measure of parameter uncertainty.

The GPR measurements considered in this example were those corresponding to the zero-offset profile (ZOP). In this case, the GPR antennae are kept in their respective wells at equal depths, and a single measurement is taken at each depth as the antennae are simultaneously lowered, yielding a data set that can be collected quickly but that does not contain as much information as if collected for two-dimensional tomographic reconstruction. One complication with multiple-offset gathers (MOG), where the antennae positions are varied such that a large number of angles pass the volume between the boreholes, is that data collection take a lot of time in relation to the infiltration processes under study.

Results of the synthetic example indicate that inversion with ZOP GPR measurements allows for accurate prediction of the soil hydraulic parameters, even with moderate noise (assumed normally distributed) present in the GPR data. While GPR measurements offer the benefit of non-intrusively monitoring changes in water saturation over large distances, measurements collected using ZOP are insensitive to lateral variations in flow. However, the combined use of ZOP measurements with local borehole saturation measurements greatly improves the accuracy and reduces the uncertainty of parameter estimates (see Figure 5).

A main limitation in this example, but not in the approach itself, lies in the assumption that the permeability is the only non-uniform parameter, since in reality additional flow parameters can be non uniform. (It should be noted that information describing the spatial variability of soil hydraulic parameters is limited.) Additionally, it was assumed that the spatial correlation patterns of log permeability were known, as was the petrophysical model. The possibility of jointly estimating the parameters of the petrophysical model, using travel time measurements for arbitrary GPR antennae positions (data collection configurations other than the ZOP), and using real field data are addressed elsewhere (Kowalsky et al., 2004b).

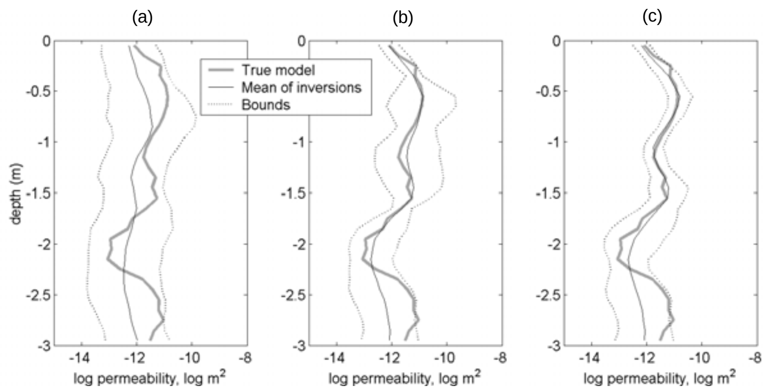

Figure 5. Vertical cross-section (within 2-D model) showing true log permeability (gray) and mean surfaces obtained from 20 inversion realizations (black lines) for (a) conditional simulation (no inversion performed), (b) inversion using only ZOP GPR measurements, and (c) inversion using ZOP GPR measurements and local borehole saturation measurements. The estimation bounds are shown with dotted lines.

1.5.3 Example 5: Fracture delineation using seismic slowness

Characterization of fractured aquifers is important for contaminant remediation and water resources investigations. Due to the complexity of fracture formations, such characterization is very challenging using conventional methods, such as borehole logging. For successful characterization, integration of multiple sources of information is often needed.

Crosshole seismic techniques have, among many other geophysical methods been found to be useful for fracture characterization. For instance, Cohen et al. (1995) showed that seismic tomography could be used to map permeable fracture zones based on data collected from the Raymond site in Virginia. Majer et al. (1997) used time-lapse seismic tomographic data before and after air injection to detect fracture channels at the Newkirk site in Oklahoma. Ellefsen et al. (2002) used seismic tomograms to map hydrogeological zonation at the Mirror Lake site in New Hampshire. Daley et al. (2003) demonstrated the potential of using seismic tomograms to monitor contaminant transport in fractured aquifers at the Idaho National Laboratory site. The main reason for the success of these examples is that seismic velocity is a function of the stiffness and density of the medium and fractures often cause a decrease of the stiffness of the medium and hence a reduction in seismic velocity.

However, in all those applications seismic travel times were first inverted and the resulting seismic velocity values were then used for hydrogeological characterization. This approach is limited for quantitative fracture characterization. First, the inverted seismic velocity is subject to uncertainty because of many reasons, such as source and receiver locations, measurement errors, deviations of boreholes, and choice of inversion methods. Second, petrophysical relations between seismic velocity and hydrogeological properties are non-unique. This is because seismic methods measure effective mechanical properties of the medium, and hydraulic behavior is not governed by the mechanical properties of the medium, although it is related (Majer et al., 1990). As indicated by many studies of fractured rock (e.g., Majer et al., 1990), only a part of the fractures are hydraulically conductive. Therefore, low seismic velocity does not necessarily correspond to high permeability.

This example is an effort to address these problems. To circumvent these limitations, Chen et al. (2003) developed a new approach to integrate crosshole seismic and borehole flowmeter data for characterizing fractured aquifers. They considered seismic travel-time (rather than inverted seismic velocity) as data and considered seismic velocity and hydrogeological zonation indicator at each pixel as unknown random variables. They used a probabilistic petrophysical model with unknown parameters to link seismic velocity to hydrogeological properties. Within a Bayesian framework, the unknown variables and parameters were simultaneously estimated using a Markov chain Monte Carlo method by conditioning to crosshole seismic travel-time and borehole flowmeter data. Data collected at the US DOE NABIR Field Research Center (FRC) at the Oak Ridge National Laboratory in Tennessee were used to test the methodology.

Figure 6 shows the estimated probabilities of being in the high permeability fracture zone along the cross-section between two wells. The red color represents high probability and the blue color represents low probability of being in the fracture zone. This image provides more information about hydrogeological zonation than using borehole flowmeter data only. If we use some cutoff value, for example 0.5 or 0.75, we can obtain an estimate of hydrogeological zonation in the fractured aquifer. We have also quantitatively compared our estimated results with the field tracer experiments, and they are consistent. For details, please see Chen at al. (2003).

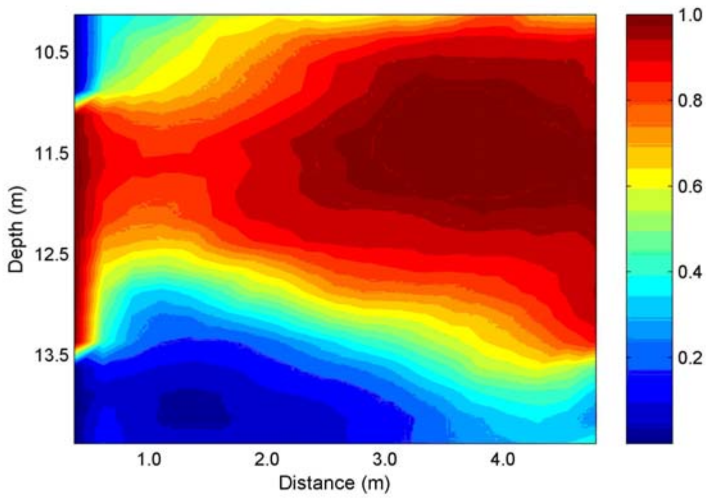

Figure 6. The probability of high permeability fracture zone along a cross section (from Chen et al., 2003).

1.5.4 Discussion of joint inversion methods

Our wide definition of joint inversion methods includes all inversions where both hydrogeological and geophysical data are used. Advantages arise in joint inversion methods compared with integration methods because well-posedness of the inverse problem generally improves when we add additional sources of information. A further advantage is that we can be very flexible in handling the petrophysical relationship within the inversion. Thus, we can test the influence of assuming a known petrophysical relationship by letting the parameters in the petrophysical relationship be free parameters in the inversion. We partially avoid scaling problems, and we can develop the petrophysical relationship at the field scale. However, we must note that measurements of hydrogeological system properties are also included in integration methods (see section 1.4) and the improvements in including them in the inversion remains to be tested. However, more fundamental improvements can be obtained through joint inversion using measurements of both geophysical and hydrogeological system variables. The reason is simply that if no measurements of dependent hydrogeological variables are included (e.g., tracer test data), all resolved structure away from measurements of hydrogeological system properties (e.g., permeability in boreholes) is due to what we resolve in the geophysical inversion. This means that we must assume stationary petrophysical relationships without any good means of testing this assumption, and we must assume that all relevant hydrogeological structure has a geophysical signature. On the other hand, measurements of hydrogeological system variables give us the opportunity to simultaneously minimize the misfit of both the hydrogeological and geophysical data.

1.6 SUMMARY AND OUTLOOK

Because geophysical data provide additional information for hydrogeological parameter estimation, even if there is uncertainty in the geophysical data and models, hydrogeophysics offers the potential for improved subsurface characterization. The choice of different methods for integrating hydrogeological and geophysical data sets largely depends on the problem. Each method is based on assumptions, which should be acknowledged and examined. No method is good for all applications at the current stage. There is much room to improve our current methods for integration as hydrogeophysics is a new and interdisciplinary field.

In this chapter, we have discussed choices that must be made in hydrogeophysical parameter estimation. We have also attempted to classify hydrogeophysical parameter estimation into three classes: direct mapping; integration methods, and joint inversion methods. We do not advocate one particular approach, but we emphasize the importance of stating our assumptions and have realistic expectations on the estimates. These expectations should be formed with regards to the available data, the goal of the study, and the hydrogeophysical parameter estimation approach. The justification of assumptions becomes very important when we want to estimate quantitative and detailed hydrogeological models, for example, that are to be used as input to flow simulations in a risk analysis.

For a quantitative analysis, we should ideally know, among other factors: the errors of our data, the intrinsic petrophysical relationships, the space-varying resolution of our individual inversions, scaling laws, the spatial correlation of different properties, discretization effects, effects of physical simplifications in the forward operators, and the small-scale variability. Naturally, sometimes the resulting estimates are relatively insensitive to errors in the description of these effects, and it might be justified to assume that we have a correct description. However, this needs to be checked, for example, by using synthetic examples or by studying similar cases in the literature.

How can fundamental improvements in hydrogeophysical parameter estimation be realized? In this work we have focused on a given data set and problem. We have discussed how we could treat uncertain petrophysical relationships, and in a qualitative manner discussed how different choices of for example objective functions or parameterization influence our estimate. We have also discussed different approaches to parameter estimation. However, careful survey design and surveying, together with a good conceptual understanding of the problem, of the petrophysical relationships, and the dominant processes are probably the most important factors in successful hydrogeophysical parameter estimation efforts. Obviously, even the most sophisticated approach cannot give a detailed estimate based on very noisy data, but it can provide reasonable error bounds. As hydrogeophysics evolves we must put more emphasis on minimizing, estimating, and parameterization of the errors in our measurements in order to improve the estimations and their uncertainty bounds. We need to improve our understanding of the validity of petrophysical relationships and maybe put more emphasis on methods that are more closely linked to groundwater flow and permeability, such as induced polarization (IP) and self-potential (SP) methods.

In conclusion, our challenge is not only to develop new parameter estimation methods, but also to make sure that the assumptions we make are valid for a given application, or at least that they do not severely bias results. We will never obtain a true model of the earth's structure, but hopefully we can obtain models that sufficiently meet our needs, even if they provide only limited information, such as bounds around the true rock properties. For this to happen, we must improve our estimations of measurement and modeling errors. We believe that approaches that we term joint inversion methods are well suited to improve error estimates, to increase our knowledge about the worth of different data types, and to design field campaigns that have the potential to give the best characterization for a given budget. However, joint inversion methods are in their infancy and the solution to many problems of practical importance can be adequately addressed using direct mapping or integration methods.

1.7 ACKNOWLEDGEMENTS

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